*
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*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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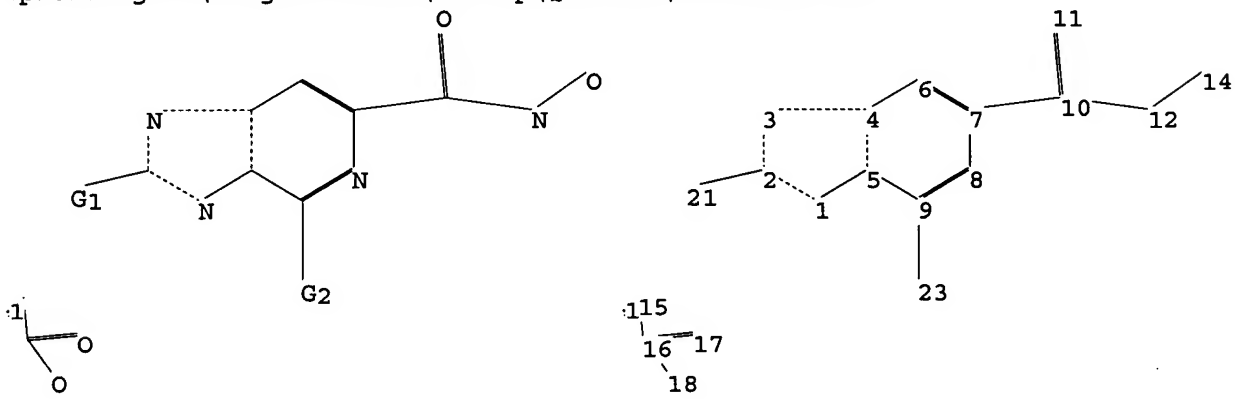

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11 14 15 16 17 18 21 23
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
10 12
chain bonds :
2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18
ring bonds :
1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9
exact/norm bonds :
1-2 1-5 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14
16-17 16-18
exact bonds :
7-10 15-16
isolated ring systems :
containing 1 :

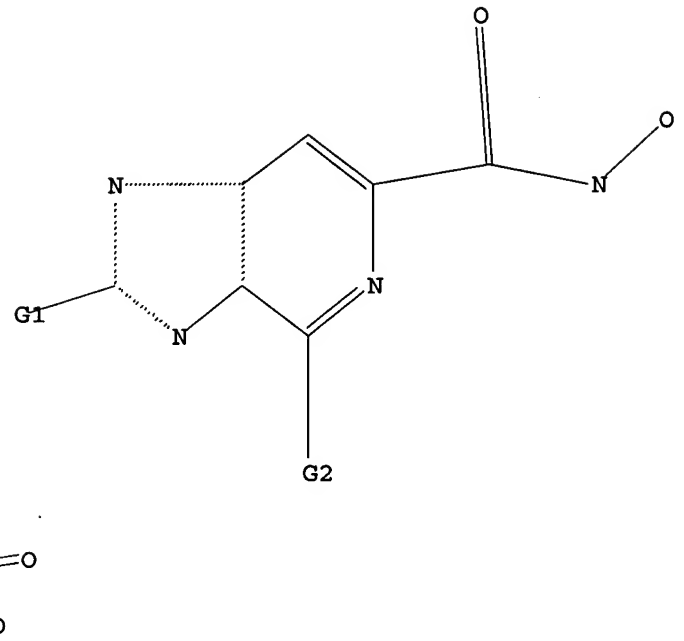
G1:H,[*1]

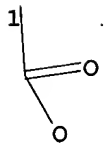
G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS
23:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR





G1 H,[@1]
G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful
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FULL SCREEN SEARCH COMPLETED - 1220 TO ITERATE

100.0% PROCESSED 1220 ITERATIONS 21 ANSWERS
SEARCH TIME: 00.00.01

L2 21 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 166.94 167.15

FILE 'CAPLUS' ENTERED AT 06:10:38 ON 28 APR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 28 Apr 2006 VOL 144 ISS 18
FILE LAST UPDATED: 26 Apr 2006 (20060426/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

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L3 2 L2

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L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1171056 CAPLUS
DN 143:440391
TI Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase.
IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewe, Michael Bruno; Tanis, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 177 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005103003	A2	20051103	WO 2005-IB1029	20050414
	WO 2005103003	A3	20060316		
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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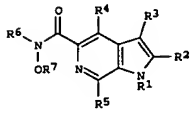
				US 2005-660502P	P 20050309

OS MARPAT 143:440391
GI

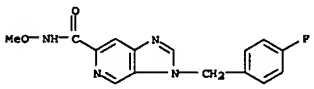


I

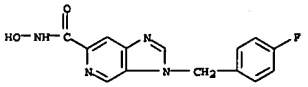
AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9)tNR10R11, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6 = H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N = (substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3], were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in DMF for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μM in an HIV-1 cell protection assay.

=> d hitstr

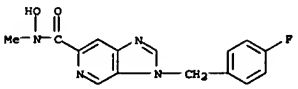
L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
IT 688314-07-0P 868550-24-7P 868550-25-8P
868550-26-9P 868550-27-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase)
RN 688314-07-0 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-methoxy- (9CI) (CA INDEX NAME)



RN 868550-24-7 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

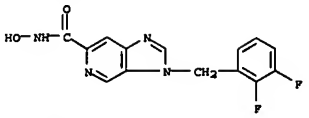


RN 868550-25-8 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-hydroxy-N-methyl- (9CI) (CA INDEX NAME)

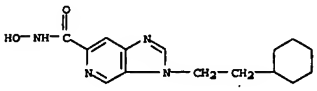


RN 868550-26-9 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,3-difluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 868550-27-0 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-hydroxy- (9CI) (CA INDEX NAME)



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L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:390246 CAPLUS
DN 140:406796
TI Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors
IN Hu, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004039803	A2	20040513	WO 2003-IB4735	20031027
WO 2004039803	A3	20040916		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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			WO 2003-IB4735	W 20031027
AU 2003269421	A1	20040525	AU 2003-269421	20031027
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			WO 2003-IB4735	W 20031027
EP 1558611	A2	20050803	EP 2003-751203	20031027
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			WO 2003-IB4735	W 20031027
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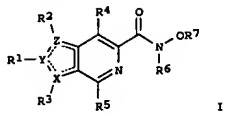
			US 2002-422513P	P 20021031
			WO 2003-IB4735	A 20031027
JP 2006506398	T2	20060223	JP 2004-547905	20031027
			US 2002-422513P	P 20021031
			WO 2003-IB4735	W 20031027
US 2004147547	A1	20040729	[redacted]	20031030
			US 2002-422513P	P 20021031
NL 1024676	A1	20040506	NL 2003-1024676	20031031
NL 1024676	C2	20051214		
			US 2002-422513P	P 20021031

OS MARPAT 140:406796
GI



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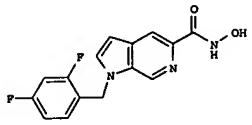
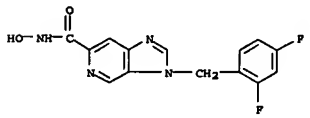


II

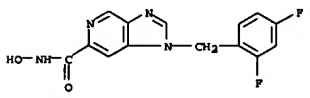
AB Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc = halo, H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, alkynyl, heteroalkyl, (hetero)cycloalkyl, or (hetero)aryl; X = C or N; Y = C or N; Z = C or N; or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof] were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions, such as AIDS (no data). Examples include 31 synthetic prepns. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addnl. prepns. of bicyclic hydroxamates without data, bioassays for HIV-integrase activity and HIV-1 cell protection without data. For instance, Et 1H-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NaH in DMF to give the N-alkylated pyrrolopyridinecarboxylate (48%). Saponification with NaOH in MeOH provided the acid (55%), which was treated with HONH2•HCl in the presence of HATU and TEA to afford (2,4-difluorobenzyl)-N-hydroxy-1H-pyrrolo[2,3-c]pyridine-5-carboxamide (II) in 48% yield.

IT **688313-86-2P**, 3-(2,4-Difluorobenzyl)-N-hydroxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688313-90-8P**, 1-(2,4-Difluorobenzyl)-N-hydroxy-1H-imidazo[4,5-c]pyridine-6-carboxamide **688314-02-5P**, N-Benzyloxy-3-(4-fluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-07-0P**, 3-(4-Fluorobenzyl)-N-methoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-08-1P**, 3-(4-Fluorobenzyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-09-2P**, 3-(4-Fluorobenzyl)-N-[(2,3,4,5,6-pentafluorobenzyl)oxy]-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-10-5P**, N-(Allyloxy)-3-(4-fluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-23-0P**, 3-(2,3-Difluorobenzyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-24-1P**, 3-(2,3-Difluorobenzyl)-N-methoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-25-2P**, N-Allyloxy-3-(2,3-difluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-26-3P**, 1-(4-Fluorobenzyl)-N-phenoxy-1H-imidazo[4,5-c]pyridine-6-carboxamide **688314-27-4P**, N-tert-Butoxy-3-(2,3-difluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-28-5P**, N-Methoxy-3-(3-methylbutyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-29-6P**, 3-(3-Methylbutyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-30-9P**, 3-(2-Cyclohexylethyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-31-0P**, 3-(2-Cyclohexylethyl)-N-methoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide **688314-32-1P**, N-Allyloxy-3-(2-cyclohexylethyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(HIV-integrase inhibitor; prepn. of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors)

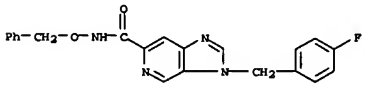
RN 688313-86-2 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,4-difluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)



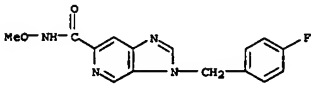
RN 688313-90-8 CAPLUS
CN 1H-Imidazo[4,5-c]pyridine-6-carboxamide, 1-[(2,4-difluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)



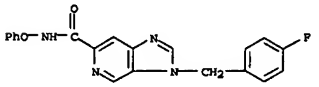
RN 688314-02-5 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-(phenylmethoxy)- (9CI) (CA INDEX NAME)



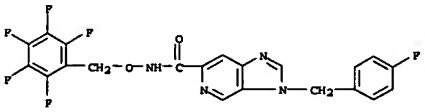
RN 688314-07-0 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-methoxy- (9CI) (CA INDEX NAME)



RN 688314-08-1 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-phenoxy- (9CI) (CA INDEX NAME)

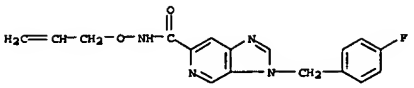


RN 688314-09-2 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-[(pentafluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

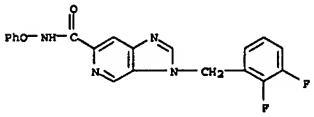


RN 688314-10-5 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-(2-propenyloxy)- (9CI) (CA INDEX NAME)

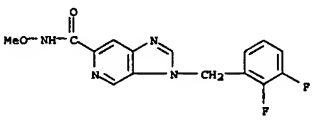
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 688314-23-0 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,3-difluorophenyl)methyl]-N-phenoxy- (9CI) (CA INDEX NAME)

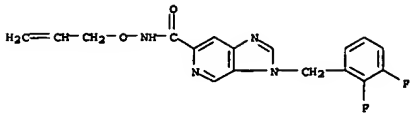


RN 688314-24-1 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,3-difluorophenyl)methyl]-N-methoxy- (9CI) (CA INDEX NAME)

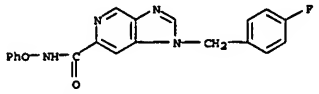


RN 688314-25-2 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,3-difluorophenyl)methyl]-N-(2-propenyloxy)- (9CI) (CA INDEX NAME)

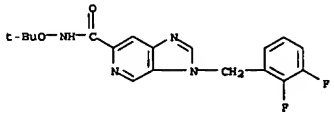
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



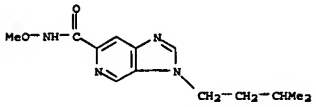
RN 688314-26-3 CAPLUS
CN 1H-Imidazo[4,5-c]pyridine-6-carboxamide, 1-[(4-fluorophenyl)methyl]-N-phenoxy- (9CI) (CA INDEX NAME)



RN 688314-27-4 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,3-difluorophenyl)methyl]-N-(1,1-dimethylethoxy)- (9CI) (CA INDEX NAME)

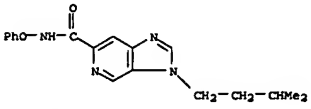


RN 688314-28-5 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, N-methoxy-3-(3-methylbutyl)- (9CI) (CA INDEX NAME)

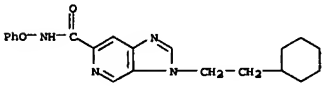


RN 688314-29-6 CAPLUS

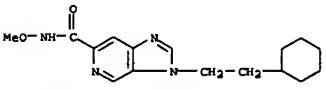
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(3-methylbutyl)-N-phenoxy- (9CI) (CA INDEX NAME)



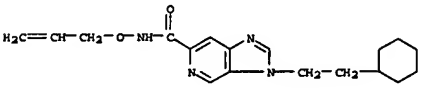
RN 688314-30-9 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-phenoxy- (9CI) (CA INDEX NAME)



RN 688314-31-0 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-methoxy- (9CI) (CA INDEX NAME)



RN 688314-32-1 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-(2-propenyloxy)- (9CI) (CA INDEX NAME)



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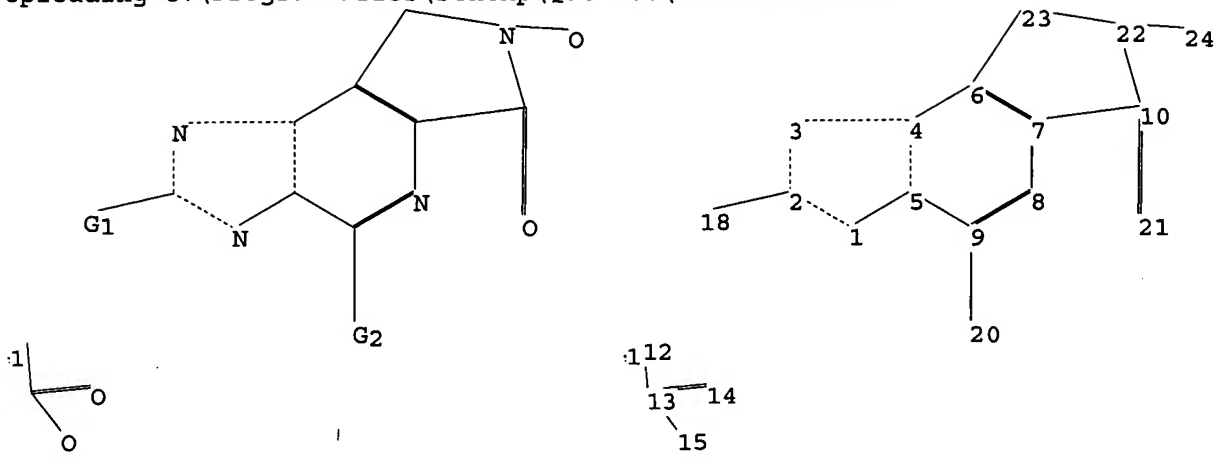

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12 13 14 15 18 20 21 24
ring nodes :
1 2 3 4 5 6 7 8 9 10 22 23
chain bonds :
2-18 9-20 10-21 12-13 13-14 13-15 22-24
ring bonds :
1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 6-23 7-8 7-10 8-9 10-22 22-23
exact/norm bonds :
1-2 1-5 2-3 2-18 3-4 4-6 4-5 5-9 6-7 6-23 7-8 7-10 8-9 9-20 10-21
10-22 13-14 13-15 22-23 22-24
exact bonds :
12-13
isolated ring systems :
containing 1 :

G1:H,[*1]

G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS 20:CLASS 21:CLASS 22:Atom
23:Atom 24:CLASS

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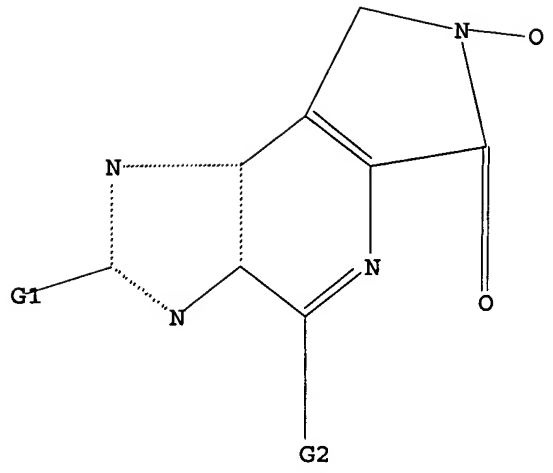
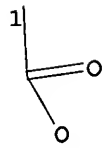
=> d
L4 HAS NO ANSWERS
L4 STR





G1 H,[@1]

G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l4 ful
REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 06:13:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 35 TO ITERATE

100.0% PROCESSED 35 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L5 0 SEA SSS FUL L4

L6 0 L5

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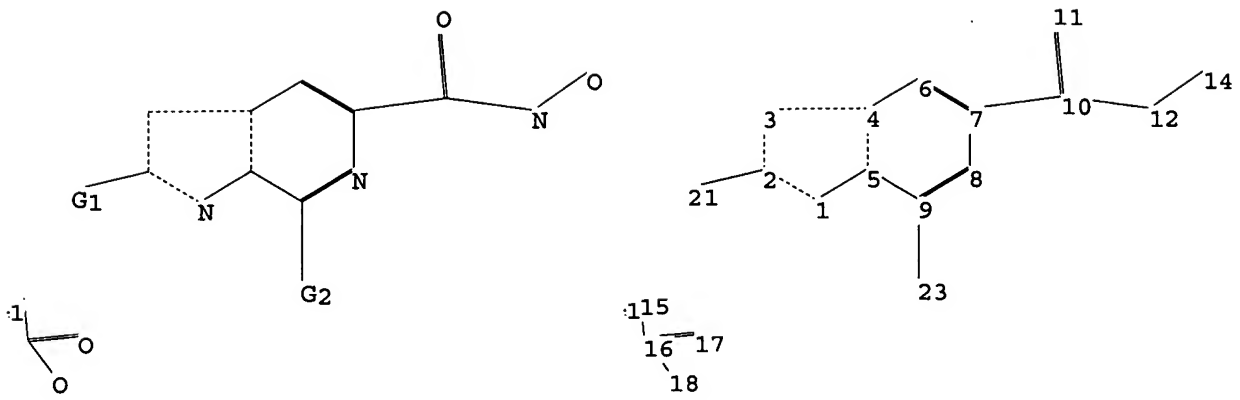


chain nodes :
11 14 15 16 17 18 21 23
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
10 12
chain bonds :
2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18
ring bonds :
1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9
exact/norm bonds :
1-2 1-5 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14
16-17 16-18
exact bonds :
7-10 15-16
isolated ring systems :
containing 1 :

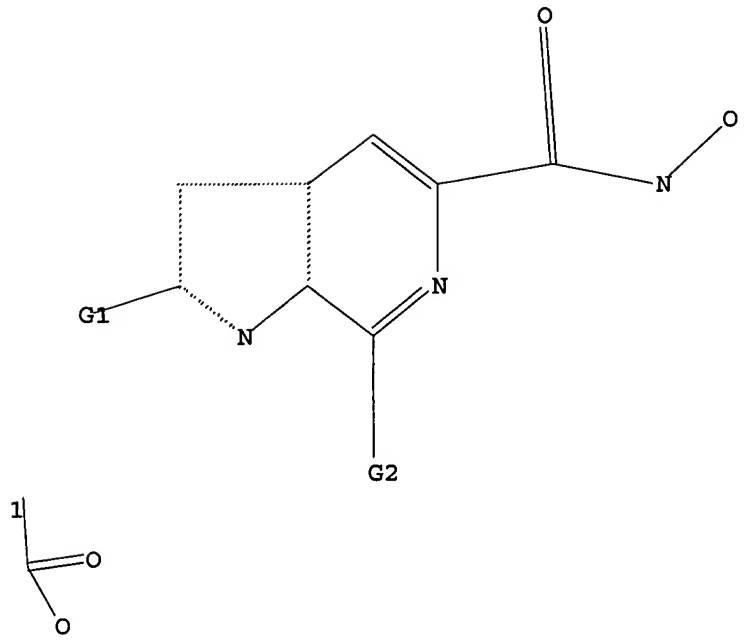
G1:H,[*1]

G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS
23:CLASS

L7 STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7 STR



G1 H,[@1]

G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l7 ful
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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FULL SCREEN SEARCH COMPLETED - 1216 TO ITERATE

100.0% PROCESSED 1216 ITERATIONS 202 ANSWERS
SEARCH TIME: 00.00.02

L8 202 SEA SSS FUL L7

L9 4 L8

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L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2006:237568 CAPLUS
DN 144:312070
TI Preparation of N-hydroxy pyrrolopyridinecarboxamides as inhibitors of HIV integrase.
IN Dress, Klaus; Kuehler, Jon Edward; Plewe, Michael Bruno; Yang, Anle; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006027694	A1	20060316	WO 2005-IB2967	20050826
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
			US 2004-607791P	P 20040907

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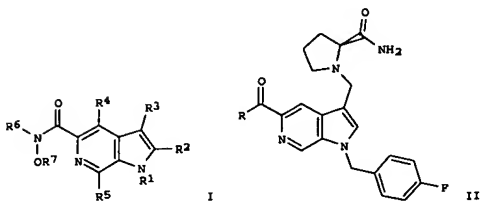

I

II

AB Title compds. I [wherein R1, R6 = H, (substituted) alkyl, alkenyl, etc.; R2, R5 = H; R3 = pyrrolidinylmethyl, piperidinylmethyl, etc.; R4 = H, halo, alkyl, etc.; R7 = H, heteroalkyl, aryl, etc.] and pharmaceutically acceptable salts and solvates thereof were prepared as inhibitors of HIV integrase. For instance, condensation of Me ester II (R = OMe) with hydroxylamine at ambient temperature gave hydroxyamide II (R = NHOH) in 15%

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
yield. The invented compds. are useful for the treatment of diseases mediated by HIV, such as AIDS and AIDS related complex.
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d fbib abs 2

L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1171056 CAPLUS
DN 143:440391
TI Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase.
IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewe, Michael Bruno; Tanis, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 177 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005103003	A2	20051103	WO 2005-IB1029	20050414
WO 2005103003	A3	20060316		
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
			US 2004-565705P P	20040426
			US 2005-660502P P	20050309
US 2005277662	A1	20051215	US 2005-115003	20050425
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			US 2005-660502P P	20050309

OS MARPAT 143:440391
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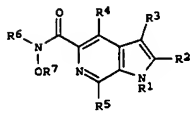

I

AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9)tNR10R11, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6 = H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N = (substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3], were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in DMF for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μM in an HIV-1 cell protection assay.

=> d fbib abs 3

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1170952 CAPLUS
DN 143:440390
TI Preparation of pyrrolonaphthyridinones, pyranopyrrolopyridinones, and pyrrolopyridoazepinones as inhibitors of HIV integrase.
IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewe, Michael Bruno; Tanis, Steven Paul; Zhu, Huichun; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005103051	A1	20051103	WO 2005-IB976	20050413
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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				US 2005-643316P	P 20050111
				US 2005-657594P	P 20050228
				US 2005-660430P	P 20050309
	US 2005277661	A1	20051215	US 2005-114813	20050425
				US 2004-565728P	P 20040426
				US 2005-643316P	P 20050111
				US 2005-657594P	P 20050228
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OS MARPAT 143:440390
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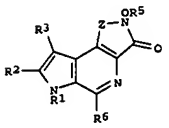

I

AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2 = H, alkyl; R3 = H, alkyl, (substituted) heteroalkyl, aminoalkyl, aminocarbonyl, etc.; Z = [C(R4)2]n, CR4:CR4, etc.; R4 = H, halo,

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
heteroalkyl, (substituted) alkyl, cycloalkyl, aryl, heteroalkyl, cycloheteroalkyl; R5 = H, heteroalky, aryl, alkenyl, (substituted) alkyl; R6 = H; n = 1-4], were prepd. Thus, 3-(4-fluorobenzyl)-7-hydroxy-3,7-dihydro-6H-pyrrolo[2,3-c]-1,7-naphthyridin-6-one (multistep prepn. given) showed EC50 = 0.4 nM in an HIV-1 cell protection assay.
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d fbib abs 4

L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:390246 CAPLUS
DN 140:406796
TI Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors
IN Hu, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004039803	A2	20040513	WO 2003-IB4735	20031027
WO 2004039803	A3	20040916		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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CA 2500487	AA	20040513	CA 2003-2500487	20031027
			US 2002-422513P	P 20021031
			WO 2003-IB4735	W 20031027
AU 2003269421	A1	20040525	AU 2003-269421	20031027
			US 2002-422513P	P 20021031
			WO 2003-IB4735	W 20031027
EP 1558611	A2	20050803	EP 2003-751203	20031027
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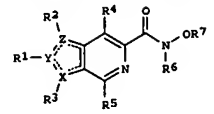
			WO 2003-IB4735	W 20031027
BR 2003015820	A	20050913	BR 2003-15820	20031027
			US 2002-422513P	P 20021031
			WO 2003-IB4735	A 20031027
JP 2006506398	T2	20060223	JP 2004-547905	20031027
			US 2002-422513P	P 20021031
			WO 2003-IB4735	W 20031027
US 2004147547	A1	20040729	US 2003-699068	20031030
			US 2002-422513P	P 20021031
NL 1024676	A1	20040506	NL 2003-1024676	20031031
NL 1024676	C2	20051214		
			US 2002-422513P	P 20021031

OS MARPAT 140:406796
GI

L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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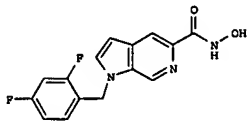

II

AB Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc = halo, H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, alkynyl, heteroalkyl, (hetero)cycloalkyl, or (hetero)aryl; X = C or N; Y = C or N; Z = C or N; or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof] were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions, such as AIDS (no data). Examples include 31 synthetic prepns. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addnl. prepns. of bicyclic hydroxamates without data, bioassays for HIV-integrase activity and HIV-1 cell protection without data. For instance, Et 1H-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NaH in DMF to give the N-alkylated pyrrolopyridinecarboxylate (48%). Saponification with NaOH in MeOH provided the acid (55%), which was treated with HONH2•HCl in the presence of HATU and TEA to afford (2,4-difluorobenzyl)-N-hydroxy-1H-pyrrolo[2,3-c]pyridine-5-carboxamide (II) in 48% yield.

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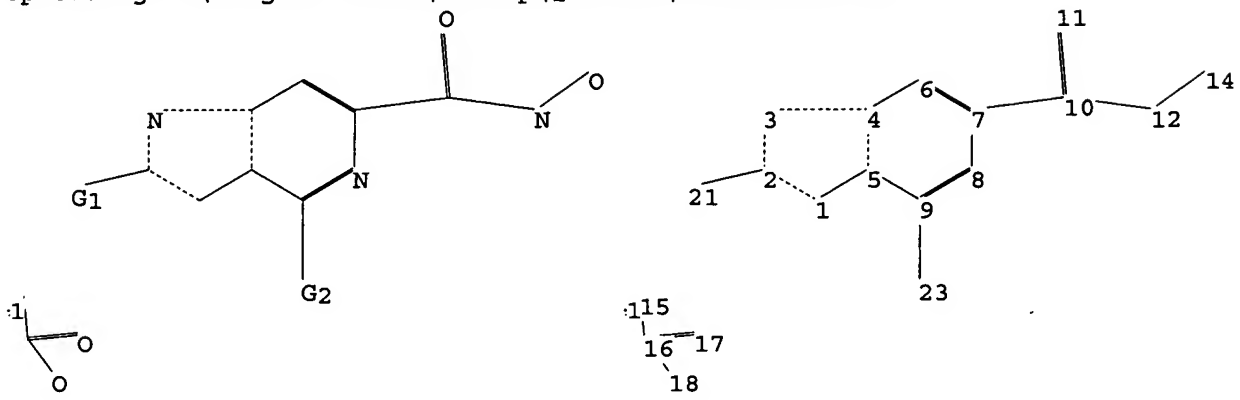


chain nodes :
11 14 15 16 17 18 21 23
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
10 12
chain bonds :
2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18
ring bonds :
1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9
exact/norm bonds :
1-2 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14 16-17
16-18
exact bonds :
1-5 7-10 15-16
isolated ring systems :
containing 1 :

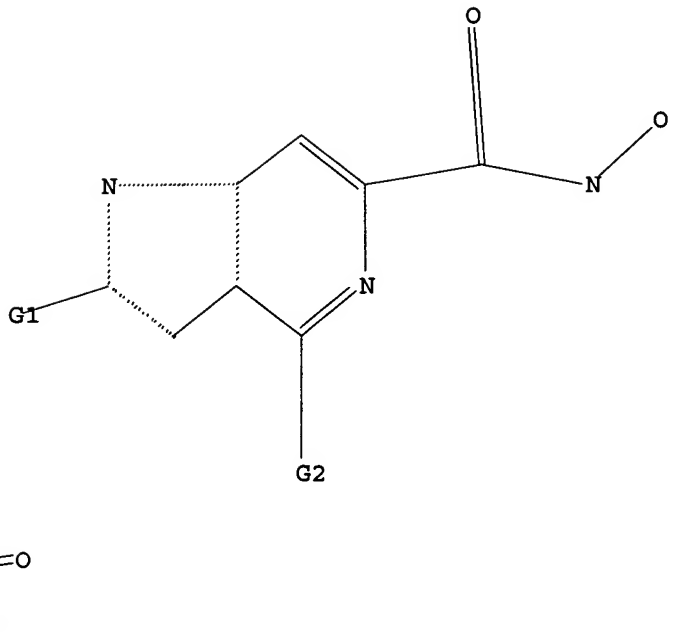
G1:H,[*1]

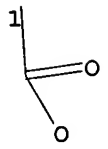
G2:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS
23:CLASS

L10 STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10 STR





G1 H,[@1]

G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

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Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 06:19:09 FILE 'REGISTRY'
SCREENING
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FULL SCREEN SEARCH COMPLETED - 1028 TO ITERATE

100.0% PROCESSED 1028 ITERATIONS 12 ANSWERS
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L12 2 L11

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L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1171056 CAPLUS
DN 143:440391
TI Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase.
IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewe, Michael Bruno; Tanis, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 177 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005103003	A2	20051103	WO 2005-IB1029	20050414
WO 2005103003	A3	20060316		

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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			US 2005-660502P	P 20050309
US 2005277662	A1	20051215	US 2005-115003	20050425
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OS MARPAT 143:440391
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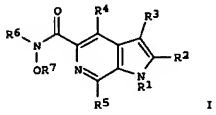

I

AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9)tNR10R11, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6 = H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N =

L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3], were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in DMF for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μM in an HIV-1 cell protection assay.

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L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:390246 CAPLUS
DN 140:406796
TI Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors
IN Hu, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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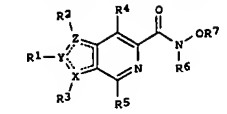
OS MARPAT 140:406796
GI

L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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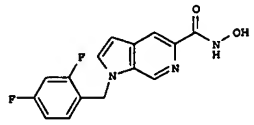

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AB Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc = halo, H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, alkynyl, heteroalkyl, (hetero)cycloalkyl, or (hetero)aryl; X = C or N; Y = C or N; Z = C or N; or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof] were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions, such as AIDS (no data). Examples include 31 synthetic prepns. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addnl. prepns. of bicyclic hydroxamates without data, bioassays for HIV-integrase activity and HIV-1 cell protection without data. For instance, Et 1H-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NaH in DMF to give the N-alkylated pyrrolopyridinecarboxylate (48%). Saponification with NaOH in MeOH provided the acid (55%), which was treated with HONH2•HCl in the presence of HATU and TEA to afford (2,4-difluorobenzyl)-N-hydroxy-1H-pyrrolo[2,3-c]pyridine-5-carboxamide (II) in 48% yield.